User manual

Toolbox 4.4 Release Notes

Document history

Version	Comment
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If you have questions or comments that relate to this document, please send them to ehscont@oecd.org or visit the QSAR Toolbox discussion forum at https://community.oecd.org/community/toolbox_forum

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1 Overview

The Toolbox 4.4 installation is a major update of Toolbox 4.3. It can be installed as a separate product alongside previous major releases of Toolbox (4.3, 4.2, 4.1, 4.0, 3.4, 3.3, etc.)

2 System Requirements

Minimum system requirements

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OS: 64 bit, Windows 7 or newer

CPU: Core 2 duo at 2 GHz or equivalent AMD CPU

RAM: At least 4GB of RAM

HDD: 14 GB free hard drive space

File system: NTFS

Microsoft .NET Framework 4.5.1

Recommended system requirements

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OS: 64 bit, Windows 7 or newer

CPU: I5 at 2.4GHz or faster processor or equivalent AMD CPU

RAM: 6 GB of RAM

HDD: 20 GB free hard drive space

File system: NTFS

Microsoft .NET Framework 4.5.1

3 Change log

I. General

- New Simplified Toolbox interface
- Development of a Toolbox web repository where different modules which could be docked to Toolbox are stored
- Development of Toolbox repository client within the QSAR Toolbox which manages the docking of external modules via direct connection to web repository or uploading from the local computer
- Possibility to "unlock" the ECHA REACH database export in Toolbox which allows exporting of data after accepting the terms and condition for usage.
- One working mode – only 2.5D mode available

II. Input

- Define target endpoint:
  - ECHA REACH endpoints could be defined
  - New options for easier definition of the target endpoint – "Define here", Copy-Paste defined target endpoint.
- Loading of list with SMILES (or CAS) shows in a window all substances corresponding to the entered identifier

III. Profiling

71 profilers (Predefined: 5; General Mechanistic: 29; Endpoint Specific: 25; Empiric: 9; Toxicological: 1; Custom: 2) and 16 metabolisms (5 observed and 11 simulated) are available.

- New "QSAR domain query" in the profiling editor.

A. New profilers

1. *Custom profile: Skin sensitization for DASS*

B. Updated profilers

1. *Acute Oral Toxicity*

2. *Biodeg Probability (Biowin 5)*
3. *Biodeg Probability (Biowin 6)*
4. *Carcinogenicity (genotox and nongenotox) alerts by ISS*
5. *DART scheme*
6. *DNA binding by OASIS*
7. *DNA alerts for AMES, CA and MNT by OASIS*
8. *Hydrolysis Half life (pH 6.5 - 7.0)*
9. *in vitro mutagenicity (Ames test) alerts by ISS*
10. *in vivo mutagenicity (Micronucleus) alerts by ISS*
11. *Organic Functional groups*
12. *Organic Functional groups (nested)*
13. *Organic functional groups (US EPA)*
14. *Protein binding alerts for Chromosomal aberration by OASIS*
15. *Protein binding alerts for skin sensitization by OASIS*
16. *Protein binding by OASIS*
17. *Protein binding potency by GHS*
18. *Substance type*

C. Updated simulators

1. *Autoxidation simulator*
2. *Hydrolysis simulator (neutral)*
3. *in vivo Rat metabolism*
4. *Microbial metabolism simulator*
5. *Rat liver S9 metabolism simulator*
6. *Skin metabolism simulator*

IV. Data

57 databases with **92 134 substances** and **2 634 458 data points** are available

- IUCLID – new options when import/export data

A. Updated databases

1. *Aquatic Japan MoE*
   - Available: 664 substances and 4 577 data points
   - New: 5 substances and 14 data points.
2. *ECHA REACH* (formerly ECHA CHEM)

- Available: 13 305 substances and 802 230 data points
- New: 1 562 substances and 133 926 data points

3. *ECOTOX*
   - Available: 11 822 substances and 969 352 data points
   - New: 167 substances and 52 306 data points
4. *Genotoxicity OASIS*
   - Available: 8 031 substances and 30 943 data points
   - New: 46 substances and 496 data points
5. *pKa OASIS*
   - Available: 2 898 substances and 3 492 data points
   - New: 968 substances and 1 183 data points
6. *Repeated Dose Toxicity HESS*
   - Available: 745 substances and 485 842 data points
   - New: 45 substances and 45 446 data points
7. *Toxicity Japan MHLW*
   - Available: 390 substances and 3 971 data points
   - New: 138 substances and 1 057 data points

B. Updated inventories

1. NICNAS
- Available: 40 180 substances
- New: 486 substances

V. Category definition

- New clustering options
- Option to sort chemicals when defined a category based on their structural similarity to the target

VI. Data Gap Filling

- New AW for Skin sensitization for Defined approaches purposes
- Implementation of the latest EPISUITE models versions

VII. <u>Reporting/Exporting</u>

- New section with all options for export in the Report module
- New template of exporting profiling result when applying export of the data matrix
- New RAAF templates for environmental and ecotoxicity endpoints
- Addition of QSAR predictions in the Data matrix report.

VIII. IT improvements

- Data matrix responsiveness improvement
- Database deployment consistency checking
- Reduced memory use on server
- Acceleration of:
    - Starting the program
    - Clustering
    - Automated workflows
    - Profiling

IX. Additional new features

- Providing numbers of chemicals, available data and predictions for each list in the document tree
- Option for removing the chemicals without experimental data on the data matrix
- Option for searching information in the data matrix
- Freezing target chemical column
- Possibility to edit an entered substance with composition
- Highlights - the row of the document tree where a prediction is accepted; sections in the report containing RAAF assessment elements.
- Improved biological taxonomy
- Caching of generated metabolites in Toolbox database (new combination of metabolic simulators and databases are cached)
- Other small improvements

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